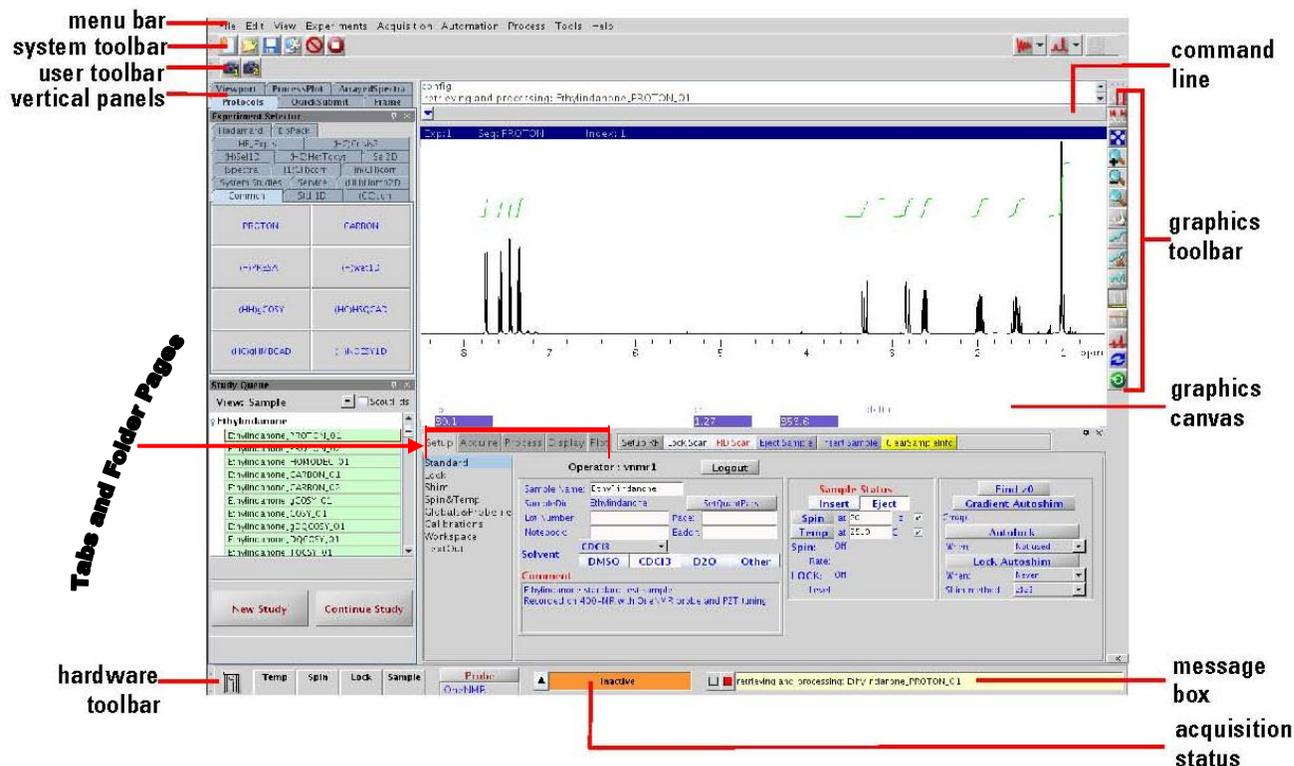# VnmrJ 3.2 Manual

This brief manual is used for running the Varian 300 MHz instrument in NMR facility

1.   LOGON   Login your account by selecting your user name, click the "**VnmrJ**" icon on the desktop to start VnmrJ.

2.   EXCHANGE SAMPLE

(1). REMOVE LOCK SAMPLE (or PREVIOUS SAMPLE)

There is ALWAYS a sample (sealed NMR sample tube, $CDCl_3$) in the magnet with the lock ON at a level of 50%-70%. Go to "**folder tabs and pages**", select **Start** (gray), then Click on **Lock** (gray) on subpanel. Click on "**Lock off**" and "**Spin off**", then Click "**Eject**" button.

Remove the sample from the top of the magnet by holding onto the top of the spinner. Then remove the previous sample from the spinner with a firm pull (twisting the sample relative to the spinner also helps) on the top end and place it at NMR samples holder.

(2). INSERT THE SAMPLE INTO MAGNET

Wipe the outside of the tube, then insert the spinner into the top of the sample depth Gauge and insert your NMR tube in to the spinner. Gently push your sample tube down until it touches the movable bottom of the sample depth gauge, put your sample into the top of upper barrel of the magnet, make sure that there is enough air to support the sample before letting go of the sample tube and spinner.

Then click "**Insert**" to let the sample descend into the probe.

3.   ESTABLISHING LOCK & SHIM

(1). Click on **Standard** (gray) on subpanel, enter your sample name in the "**Name Sample"** field. Select your sample's solvent in the "**Solvent**".
Write a note in "Comment" (optional).

(2). Click on **Lock** (gray) on subpanel, click "**Find Z0**". When acquisition status show Idle, click "**Gradient Shims**". Click spin on by clicking "**Spin On**" after acquisition status show Idle.

acquisition status

4.   MANUALLY SHIMMING

(Optional, you can skip MANUALLY SHIMMING if you click "Gradient Shims")

Click on **Shim** (gray) on subpanel. Click on "**Read1**" to load shim file. Adjust the Z1C and Z2C, then Z1 and Z2 (10, then 1) to maximize the lock level. Then, adjust **lockpower** and **lockgain** to leave the lock level at 70-80%.

5.   SET-UP EXPERIMENT

(1). Double click "**Proton"** in the locator protocol list (left side of interface) or open your file to load the standard proton protocol and the appropriate parameters and their values into the workspace.

(2). Go to "folder tabs and pages", Select **Acquire** button (gray) to check the parameters. Select **Spectral width,** and **Number of scans** based on your sample's concentration.

6.   COLLECT SPECTRUM

Click on Acquire button (green) to acquire NMR data. Or Type "**go**" or "**ga**" at the VnmrJ command line to start acquisition.

7.   DATA PROCESSING

After acquisition (when acquisition status show Idle), Go to "folder tabs and pages", click on **Process.** Type "**aph**" to do automatic phase correction. If spectrum is not well phased using autophase, you also

can do manually phase. Click on phasing tool icon. Click left mouse button on a peak on right of spectrum. Sliding mouse while holding left or right button will adjust phase on the selected peak. This is the zero-order phase (rp). Move mouse to peaks at left of spectrum and click left button. Sliding mouse while holding left or right button will adjust phase in this region of the spectrum while leaving the initial peak as before. This is the first order phase correction (lp).

To reference the spectrum:

Place a cursor on your reference signal (TMS or solvent), type "**nl**" and press enter, then go to **Display->More** and input the reference frequency and click on "**Reference Now"** or type "**rl**" to set the reference chemical shift.

To peak picking:

Go to **Display-Line list**, click the "**Set threshold**" button, you will see a horizontal cursor appear on the screen. Drag it with the left mouse button to an appropriate threshold level.

To integrate the spectrum:

Go to **Display->Curors/Integration**, click "**AutoRegion**" to select integrals. For selecting integral regions manually, click on integral tool, which will spawn additional integral icons. Click "**2nd integral icon**", the left mouse button will choose integral reset points. Click left mouse button at the left end of a peak to be integrated then click the left mouse button just to the right of the peak. This defines the integral region for that peak. Do the same for all peaks or regions of interest. Type "**setint(int, value**) to normalize the integration. Int is the integral.

To plot the spectrum:

Type "**vp=12 pl pscale pap ppf pir page**" to print your spectrum. Based on your requirement, you can delete any options. "**pscale**": plot scale, "**pap**": plot parameters, "**ppf**" plot peak picking, "**pir**": plot integration. Or select File->Auto Plot or Print Screen

8. SAVE SPECTRUM

Type "**pwd**" to print the current working directory. Change to your own directory using "**cd('/your directory/')**" command, then type "**svf('filename')** " to save the data.

9. PUT STANDARD SAMPLE BACK

Go to "**folder tabs and pages**", select **Start** (gray), then Click on **Lock** (gray) on subpanel. Click on "**Lock off**" and "**Spin off**", then Click "**Eject**" button, move your sample, put standard sample at the top of the magnet, then, click "**insert**" button to let the sample descend into the probe, click "**Find Z0**" to lock on the standard sample.

10. LOGOFF

Type "**exit**" on the command line to logout VNMR or select **File-> exit vnmrj**, **Do not use X out!!** Then select **System-> logout your account**.